

The DOE Center of Excellence for The Synthesis and Processing of Advanced Materials



Basic Energy Sciences
Division of Materials Sciences and Engineering

Center Projects

- Start and Graduation Dates
- Projects Descriptions

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Center Projects

Start and Graduation Dates



Basic Energy Sciences
Division of Materials Sciences and Engineering

<u>Project</u>	<u>Start</u>	<u>Graduation</u>
• Metals Forming *	FY'94	FY'00
• Materials Joining	FY'94	FY'99
• Microstructural Engineering with Polymers*	FY'94	FY'00
• Tailored Microstructures in Hard Magnets	FY'94	FY'99
• Processing for Surface Hardness	FY'94	FY'99
• Mechanically Reliable Surface Oxides for High-Temperature Corrosion Resistance (MRSOX)	FY'94	FY'99
• Nanoscale Materials For Energy Applications	FY'94	Discontinued in '96
• High Efficiency Photovoltaics	FY'97	FY'01
• Design and Synthesis of Ultrahigh-Temperature Intermetallics	FY'98	FY'02
• The Science of Localized Corrosion	FY'99	FY'03

* Restructured in 1995

Center Projects

Start and Graduation Dates



Basic Energy Sciences
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<u>Project</u>	<u>Start</u>	<u>Graduation</u>
• Interfacial Adhesion Related to Protective Oxides Grown on Metallic Substrates **	FY'00	FY'01
• Isolated and Collective Phenomena in Nanocomposite Magnets	FY'00	FY'04
• Controlled Defect Structures in Rare-Earth Ba-Cu-O Cuprate Superconductors	FY'00	FY'04
• Smart Structures Based on Electroactive Polymers	FY'01	FY'05
• Nanoscale Phenomena in Perovskite Thin Films	FY01	FY'05
• Granular Flow and Kinetics	FY'02	FY'06
• Synthesis and Processing of Carbon-Based Nanostructured Materials	FY'02	FY'06
• Experimental & Computational Lubrication at the Nanoscale	FY'03	FY'07
• Spin-Polarized Transport in Complex Oxide	FY'04	FY'08

** Two-Year follow-on Project to ---- MRSOX

Objectives

- *Develop a scientific understanding of the phenomena relating to the forming of aluminum alloys for industrial (especially automotive) applications.*

Tasks

- Dynamics of Dislocation Substructure
- Particle-Stimulated Recrystallization
- Constitutive Equations for Hot Rolling

Focus: Al-Mg and Al-Cu Alloys

Participants

- Ames, LBNL, LLNL, LANL, ORNL, PNNL, SNL/CA, SNL/NM, UI/MRL, Cornell, Oregon State

Coordinator

- Michael Kassner, Oregon State, (541) 737-7023

Sponsoring/Collaborating Organizations

BES/DMS**EE/OTT****DP****Alcan****Reynolds Aluminum**

Objectives

- *Improve the reliability of the processes used to join materials into more complex structures serving a variety of energy-related functions.*

Tasks

- The Effects of Gradients on Weld Reliability and Performance *Focus: Al-Cu and Fe-Ni-Cr Alloys*
- Ceramic and Dissimilar Materials Joining *Focus: Joining SiC and SiC-based CFCCs*

Participants

- Ames, INEEL, LBNL, LLNL, ORNL, PNNL, SNL/CA, SNL/NM

Coordinator

- R. Bruce Thompson, Ames, (515) 294-8152

Sponsoring/Collaborating Organizations

BES/DMS

FE/AR

EE/OTT

EE/OIT

DP

Microstructural Engineering with Polymers



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Objectives

- *Develop and implement novel processing methods which direct the evolution of hierarchical microstructures in composites, impart multifunctionality, and induce property changes through blending of components at the molecular level.*

Tasks

- Engineered Porosity

*Focus: *Surfactant-Templated
Ceramic Phases
Inorganic Polymer Membranes

- Blends, Composites, Alloys

*Focus: *Conducting Polymers
*Polymer Molecular Composites
Polymer Blend Miscibility

Participants

- Ames, ANL, BNL, INEEL, UI/MRL, LBNL, LLNL, ORNL, PNNL, SNL/NM

Coordinator

- Gregory J. Exarhos, PNNL, (509) 375-2440

Sponsoring/Collaborating Organizations

**BES/DMS EE/OIT EE/OTT Armstrong World Ind. Advanced Battery Consortium
Power Conversion Inc. Gould Electronics Technochem, Inc. Hoechst-Celanese**

Tailored Microstructures in Hard Magnets



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Objectives

- *Improve hard magnets by understanding, in terms of the microstructures achieved, the magnetic and mechanical properties of materials produced by a number of synthesis and processing approaches.*

Tasks

- Synthesis: Powders, Compacts, Single Crystals, Thin Films.
- Characterization: Magnetic and Structural Properties.
- Theory and Modeling

Focus: $Nd_2Fe_{14}B$ as a Model System; Novel SmCo-based Systems

Participants

- Ames, ANL, BNL, INEEL, LBNL, LLNL, LANL, ORNL

Coordinator

- Robert Dunlap, ANL, (630) 252-4925

Sponsoring/Collaborating Organizations

BES/DMS

EE/OTT

DP

Consortium for Advanced Magnets (university/industry)

Objectives

- *Address the critical synthesis and processing issues which limit the use of plasma-based processing for improved surface hardness. Explore other novel approaches for achieving the same.*

Tasks

- Plasma Ion Immersion Processing (PIIP)
- Boron-Based Superhard Coatings: *Focus: cBN, Boron Suboxides*
- Tailored Microstructures for Tribological Applications:
Focus: Diamond Films, Al/O, Nanoscale Structures

Participants

- ANL, BNL, LBNL, LLNL, LANL, ORNL, SNL/CA, SNL/NM, UI/MRL

Coordinator

- James B. Roberto, ORNL, (423) 576-0227

Sponsoring/Collaborating Organizations

BES/DMS**EE/OTT****DP**

Mechanically Reliable Surface Oxides for High-Temperature Corrosion Resistance



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Objectives

- *Generate the knowledge required to establish a scientific basis for the design and synthesis of improved (slow growing, adherent, sound) protective oxide coatings and scales on high temperature materials without compromising the requisite bulk material properties.*

Tasks

- Substrate/Protective Oxide Interactions.
- Prediction of Scale/Coating Failure.
- Requirements for Improved Scales/Coatings.

Focus: Alumina Scales and Coatings

Participants

- ANL, INEEL, LBNL, LLNL, ORNL

Coordinator

- Linda L. Horton, ORNL, (423) 574-5081

Sponsoring/Collaborating Organizations

BES/DMS

FE/AR

EPRI

High Efficiency Photovoltaics



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Objectives

- *Generate advances in scientific understanding that will impact the efficiency, cost and reliability of thin film photovoltaics cells by addressing the short- and long-term basic research issues.*

Tasks

- Silicon-Based Thin Films
- Next-Generation Thin Film Photovoltaics:

Focus: Multijunction cell with $\geq 40\%$ efficiency

Participants

- Ames, ANL, BNL, LBNL, NREL, ORNL, PNNL, SNL/NM, SNL/CA, Caltech, Iowa State U., U. of Calif. (Santa Barbara), MIT, U. of IL, U. of FL, Wash. St. U., SUNY Buffalo, U. of UT

Coordinators

- Satyen K. Deb/J. Benner, NREL, (303) 384-6405, satyen_deb@nrel.gov

Sponsoring/Collaborating Organizations

BES/DMS

EE/Photovoltaics

EPRI

Design and Synthesis of Ultrahigh-Temperature Intermetallics



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Objectives

- *Generate the knowledge required to establish a scientific basis for the design and processing of transition-metal silicides and materials based on silicides for structural applications at temperatures of 1400°C and above.*

Tasks

- First Principles Calculations/Simulations
- Structure and Properties
- Processing and Fabrication

Focus: Mo₅Si₃-base Alloys

Participants

- Ames, ANL, INEEL, LBNL, LLNL, LANL, ORNL, SNL/CA, UI/MRL

Coordinators

- R. Judkins, ORNL, (423) 574-4572/R. B. Thompson, Ames

Sponsoring/Collaborating Organizations

BES/DMS

FE/AR&TD

EE/AIM

The Science of Localized Corrosion



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Objectives

- *Advance the fundamental understanding of the mechanisms leading to the initiation, propagation and cessation of localized corrosion of aluminum and its alloys to permit accurate life predictions and intelligent designs.*

Tasks

- Oxide structure and chemistry
- Metallurgical factors
- Localized chemistry and electrochemistry

Participants

- Ames, BNL, LLNL, PNNL, SNL, UI/FSMRL, Ohio State, U. Utah, U. Virginia

Coordinator

- Kevin Zavadil, SNL (505) 845-8442, krzavad@sandia.gov

Sponsoring/Collaborating Organizations

**BES/DMS&EDP EE/OTT Office of Radioactive Waste Management, NRL, Alcoa,
Ford, Lucent Technologies**

Interfacial Adhesion Related to Protective Oxides Grown on Metallic Substrates



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Objectives

- *Further the fundamental understanding of the interfacial bonding and dynamics that underlie oxide-metal adhesion and the energetics associated with decohesion for systems relying on protective alumina through theoretical calculations, experimentation and modeling.*

Tasks

- Nature of bonding at oxide interfaces and the effects of segregants
- Stress measurements, microstructure and modeling of diffusion-induced stress generation
- Modeling of pore formation and interaction

Participants

- ANL, INEEL, LBNL, ORNL

Coordinator

- Linda Horton/Peter Tortorelli, ORNL (423) 574-5081, hortonll@ornl.gov

Sponsoring/Collaborating Organizations

BES/DMS&E

FE/ATS Westinghouse,

Pratt & Whitney,

Allison Engines

Isolated and Collective Phenomena in Nanocomposite Magnets



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Objectives

- *Develop improved understanding of magnetic properties and improved magnetic materials using nanoscale mixtures of hard magnets, soft magnets and non-magnetic materials.*

Tasks

- Synthesis and investigation of isolated magnetic nanoparticles
- Synthesis and investigation of collective behavior in materials with defined microstructures
- Modeling and simulation of nanoscale magnets

Participants

- Ames, ANL, BNL, INEEL, UI/FSMRL, LANL, LBNL, LLNL, ORNL and SNL

Coordinator

- Sam Bader, ANL (630) 252-4960, bader@msd.anl.gov

Sponsoring/Collaborating Organizations

BES/DMS&E

Magnequench,

Rhodia,

IBM,

Motorola,

IAP Inc.

Controlled Defect Structures in Rare-Earth-BaCu-O Cuprate Superconductors



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Objectives

- *Provide an integrated scientific understanding of lattice defects and their nanoscale structure in the “123” rare-earth cuprates, their dependence on the various methods of synthesis, and their relationship to the resulting superconducting properties.*

Tasks

- Specimen fabrication by state-of-the-art methods
- Structure and chemical characterization using advanced and specialized methods of TEM
- Electromagnetic characterization by transport, magneto-optical and local probe measurements
- Theoretical modeling including electromagnetic and flux-pinning properties of defects

Participants

- Ames, ANL, BNL, LANL, ORNL and SNL

Coordinator

- David O. Welch (516) 344-3517, dwelch@bnl.gov

Sponsoring/Collaborating Organizations

BES/DMS&E EE/HTSC, American Superconductor, Oxford Superconductor,
Intermagnetics General, Superconductive Components

Smart Structures Based on Electroactive Polymers



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Objectives

- *Develop a framework for the rational design of self-assembled nanostructured block copolymers that offer significant advantages over conventional materials for the active regulation of transport phenomena.*

Tasks

- Modeling properties at the molecular level
- Molecular architecture modeling D
- Development of synthesis and processing methods
- Structural determination and properties measurement

Participants

- Ames, ANL, BNL, UI/FSMRL, INEEL, LBNL, LLNL, ORNL, PNNL, SNL

Coordinator

- Gregory Exarhos, PNNL, (509) 375-2440, gj_exarhos@pnl.gov

Sponsoring/Collaborating Organizations

BES/DMS&E

EE/OTT

EE/Environmental Programs

Nanoscale Phenomena in Perovskite Thin Films



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Objectives

- *Develop the scientific basis for controlling nucleation, growth and strain in ferroelectric perovskite thin films.*
- *Determine the relationship between the critical electrical properties and film microstructure, strain and perovskite/substrate interfacial interactions.*

Tasks

- Controlled growth of perovskite films on silicon substrates
- Nanoscale structure-property relationships on perovskite films

Participants

- ANL, LANL, ORNL, SNL, Northwestern U., U.N. Carolina, U. Maryland, U. Florida, N. Illinois U.

Coordinators

- Orlando Auciello, ANL (630) 252-1685 auciello@anl.gov
- Duane Dimos, SNL (505) 844-6385 dbdimos@sandia.gov

Sponsoring/Collaborating Organizations

BES/DMS&E, DP, EE/OTT, Agilent, ATMI, Ionwerks, Neocera, Oxxel, Symetrix

Granular Flow and Kinetics



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Objectives

- *Close the gap between physics and engineering descriptions of cooperative effects in granular flows by bridging between continuum models and discrete models and thereby develop and understand appropriate constitutive relationships for complex flows.*

Tasks

- Dynamic constitutive relationships for granular flow (hydrodynamic and kinetic theory via statistical mechanics of large systems)
- Low-dimensional, constrained granular dynamics (granular systems with magnetic, electric and capillary forces, tethers and chain-line constraints; mapping from 2D to 3D)

Participants

- Ames, ANL, LANL, SNL/NM

Coordinator

- David Hoffman, Ames Lab (515) 294-9649
hoffman@ameslab.gov

Sponsoring/Collaborating Organizations

BES/DMS&E	DOE	Exxon Mobil	EPRI	SUNY(Buffalo)	Univ. of Chicago
MNR Inc.	Duke Univ.	Univ. of Colorado	UC/SD	UNM	

Synthesis and Processing of Carbon-Based Nanostructured Materials



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Objectives

- *Advance the science and technology of carbon-based materials through fundamental understanding of phenomena induced by micro- and nanostructuring with emphasis on technical issues that will lead to the development of new generations of Micro- and Nano-Electromechanical Systems (MEMS and NEMS).*

Tasks

- Synthesis and processing and fundamental mechanical and tribological properties
- Fundamental transport processes in nano-scale carbon-based materials

Participants

- ANL, LBNL, ORNL, SNL/NM, N. Carolina State U., Northwestern U

Coordinators

- Dieter Gruen and John Carlisle, ANL
- Tom Friedmann, SNL/NM (505) 844-6684, tafried@sandia.gov

Sponsoring/Collaborating Organizations

BES/DMS&E

DOE/DP

EERE/Transp. Tech

Experimental and Computational Lubrication at the Nanoscale



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Objectives

- *Develop a scientific understanding of lubrication and strategies to control tribology at the nanoscale capitalizing on recent advances in nanoprobe, theoretical and computational methods.*

Tasks

- Confined Water/Non-polar Fluids/Patterned Surfaces and Lubrication
- Development of New Probe Methods
- New theory and Computation Related to Experiments

Participants

- ANL, LANL, LBNL, ORNL, SNL/NM, UI/FS-MRL, UCSD

Coordinator

- Steve Granick (UI/FS-MRL), (217) 333-5720, sgranick@uiuc.edu

Sponsoring/Collaborating Organizations

BES/DMS&E

DOE/OTT

DOE/DP

Interactions w/~12 Companies

Objectives

- *Understand, control and manipulate spin-polarized transport within and between highly spin-polarized oxides in order to create and exploit spintronic functionality.*

Tasks

- Synthesis & Processing: Tailoring Interfacial Chemistry and Structure
- Spin Transport Across and Along Interfaces
- New Theory and Computation Related to Experiments

Participants

- ANL, BNL, LANL, LLNL, ORNL, UI/FS-MRL, Cornell, Univ. of Tennessee

Coordinator

- John Mitchell, ANL, (630) 252-5852, mitchell@anl.gov

Sponsoring/Collaborating Organizations

BES/DMS&E**DOE/DP****Motorola****IBM**